Chimie Electrochimie Moléculaires et Chimie Analytique
UMR CNRS 6521, University of Brest, France
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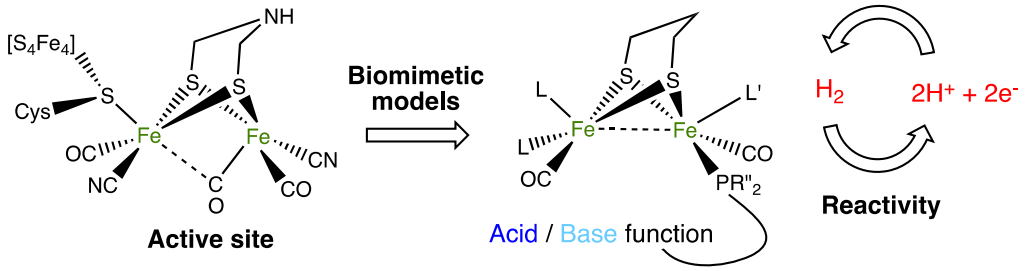
PhD research proposal

Hydrogen oxidation by Fe-based molecular complexes inspired by the [FeFe]-hydrogenase active site

From 1st Oct. 2021 to 30th Sept. 2024
In CIEL, CEMCA Laboratory, UMR CNRS 6521, University of Brest (UBO), France

Keywords: Bio-inorganic chemistry, ligands, iron, hydrogen oxidation, catalysis

Context: Sources and exploitation of green energy remains a major challenge for our society. In this context, a potential key to this issue is the utilization of hydrogen molecule as an energy driver.[1] However, catalytic systems able to reversibly activate or produce H_2 are rare. Moreover, they often are supported by noble metals, which are expensive and have a significant impact on environment. In contrast, natural iron-based enzymes, named hydrogenases, efficiently catalyze this reaction.[2] Inspiration from nature can be taken to develop cheap and abundant iron catalysts for H_2 production and oxidation.[3,4] This research project proposed to target the syntheses of iron complexes mimicking [FeFe]-hydrogenase active site to study their properties and reactivity focusing on challenging hydrogen activation.[5] Indeed, only handful complexes are able to catalytically convert hydrogen into protons in contrast to the opposite reaction.



Summary: In order to develop novel iron-based catalysts for H_2 oxidation, the PhD student will devote the first part of the thesis to the synthesis of designed mono and dinuclear iron complexes with specific ligand. The properties of the iron species will be investigated and the reactivity with hydrogen in presence or not

of external substrates will be explored. Modulation of electronic and steric effects of the substituents on ligands will be examined to observe the impact on reactivity. Spectroscopic characterizations will be used to understand structural properties (IR, NMR...). The second step will concern the study of their electrochemical properties, notably for developing novel electrocatalysts. Theoretical calculations will be performed in Milan to further characterize the transient species and their respective stability. A short stay in Milan could be planned for the recruited PhD student.

Candidate profile: Highly motivated student holding a Master Degree in chemistry. The project is multidisciplinary combining organic ligand synthesis, coordination studies on iron complexes and reactivity studies. In consequences, experiences in both organic and inorganic syntheses under controlled inert atmosphere and spectroscopic /electrochemical characterizations will be appreciated. UBO is dedicated to promoting the role of women in science, and, therefore, explicitly invites women to apply.

Application details:

Supervisors: Dr. Lucile Chatelain (Assistant Prof., lucile.chatelain@univ-brest.fr) and Prof. Philippe Schollhammer (philippe.schollhammer@univ-brest.fr)

The PhD grant is supported by the ANR OxySplit-H2 project for 3 years starting from the 1st October 2021. Candidates should submit their application to Lucile Chatelain in one pdf file including a CV, transcript of academic records from Bachelor to Master 2, a motivation letter and contact details of two references.

Application deadline: 01/05/2021

References

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